Low-dimensionally ordered structure in metal complexes analyzed with the energy spectrum of the diffuse x-ray scattering intensity

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Recent development of synchrotron-based X-ray diffraction techniques together with modern methods of analysis, such as the maximum entropy method and resonant x-ray scattering, makes us able to discuss the electronic states of materials. In the most techniques, spatial arrangement of the atoms is observed in order to make clear the spatial arrangement of the ions having specific electronic states. It is a reasonable way for the most cases that have sufficient electron-lattice coupling. Knowledge of the local structure, which usually reflects the electronic states, is sometimes essential to understand the functions of materials. That is the reason why structure analysis has been important in solid state physics. Unfortunately, a change in local structure does not necessarily form a three-dimensional (3D) ordering. This means that most of the analyzing methods as well as ordinary structure analysis provide insufficient results to clarify the electronic states in some cases; they are based on the 3D ordering of the atomic arrangement and, therefore, do not give a low-dimensional ordering that produces no Bragg reflections but does produce diffuse X-ray scattering.

In this study, we present a powerful method of observing low-dimensional ordering of a local structure by focusing on diffuse X-ray scattering. The samples were halogen-bridged quasi-1D metal complexes, which have been known as possible materials for high-performance optical devices due to their huge third order nonlinear optical susceptibilities. One of the samples we measured here, which comprises Pt-Pt-I chain structure, attracts considerable interest for its high electric conductivity. Several types of valence arrangement in a chain are proposed for this kind of complexes in order to explain their properties, while there is no method to observe the low-dimensional structure.

Synchrotron X-ray diffraction measurements were performed at beamlines BL-1A, 1B, and 4C at the Photon Factory, KEK, Japan and at BL-02B1 at the SPring-8, Japan. Beamlines 1A and 1B have imaging-plate Weissenberg cameras. They were used for sample characterization and for observing the overall features of diffuse scattering distribution. BL-4C and BL-02B1 have standard four-circle diffractometers. They were used for the measurements of energy spectrum of diffuse intensity.

Each possible valence arrangement shown in Fig.1 produces different diffuse scattering intensity distribution. The difference is more prominent when we extract the scattered amplitude of Pt component or that of I component. We have successfully obtained the low-dimensional structure by utilizing this difference observed by the energy spectrum of the intensity nearby the Pt L_{III} and I K absorption edge. The data shown in Fig. 2 clearly shows that the CDW type structure is established in the material.

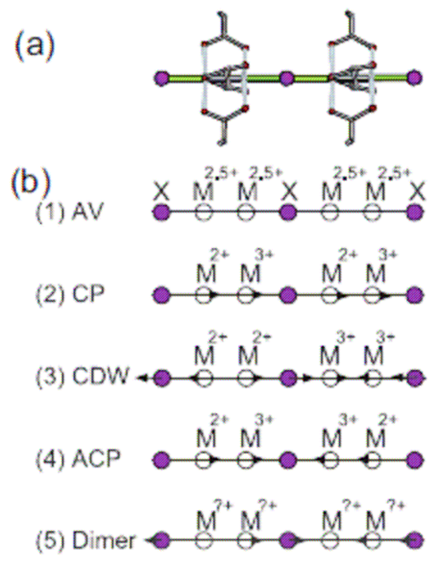

Fig.1: Schematic view of the (a) sample and (b) possible valence arrangements.

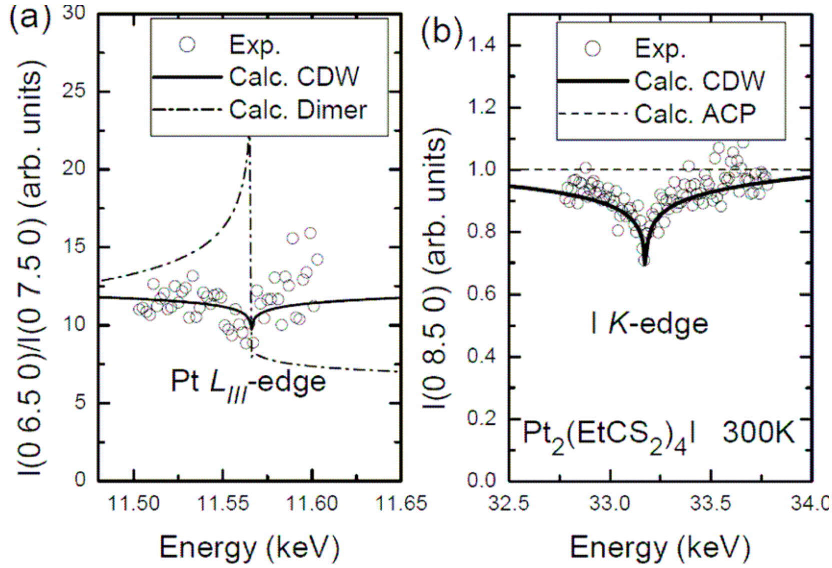

Fig.2: Energy spectrum of the diffuse intensity at (a) Pt L edge and (b) I K edge.